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Optimizing Heat Treatment Parameters for 3rd Generation AHSS Using an Integrated Experimental-Computational Framework

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2018 DOE VTO ANNUAL MERIT REVIEW
JUNE 19, 2018

PROJECT ID# MAT129

Timeline

- ▶ Project Start Date: FY16
- ▶ Project End Date: FY19
- ▶ Percent complete: 50%

Budget

- ▶ Total project funding (FY16-17)
 - DOE : \$1,100k
 - ASPPRC in-kind: \$200k
- ▶ Anticipated future funding (FY18-19)
 - DOE: \$500k
 - In-kind: \$200k

Barriers

- ▶ The traditional heat treatment (HT) and characterization process make the development-to-deployment cycle of 3rd GEN Med-Mn AHSS very long
- ▶ Lack of fundamental and quantitative understanding between alloying content, HT parameters, microstructures and associated mechanical properties of Med-Mn AHSS

Partners

- ▶ Pacific Northwest National Lab (PNNL)
- ▶ Advanced Steel Processing and Products Research Center (ASPPRC), Colorado School of Mines (CSM)
- ▶ Oak Ridge National Lab (ORNL)
- ▶ Advanced Photon Source (APS), Argonne National Lab (ANL)



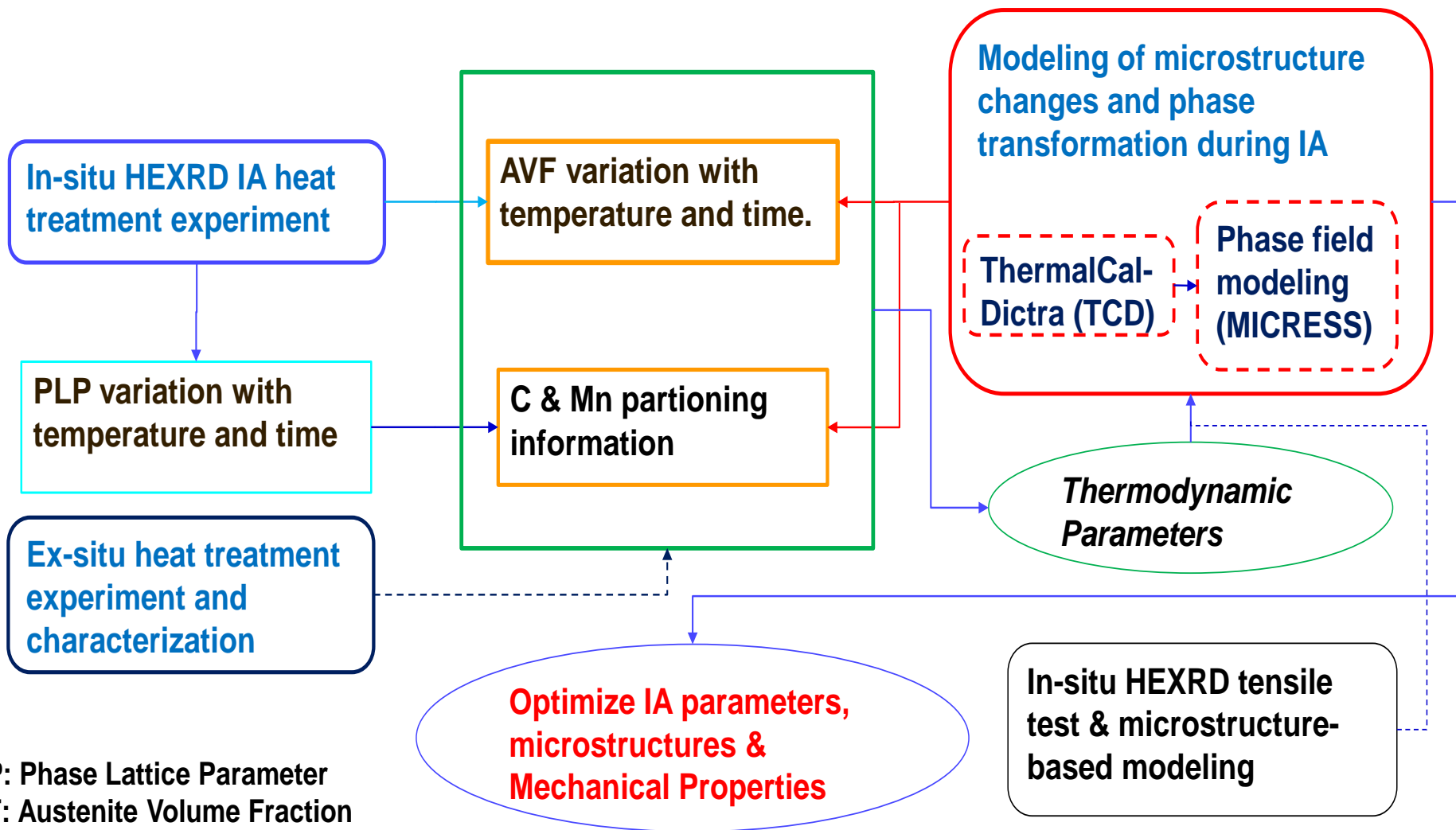
Relevance/Objectives

- ▶ Development of an integrated in-situ & ex-situ experimental and numerical modeling framework for Med-Mn 3Gen AHSS to
 - Determine accurate thermodynamic parameters.
 - Obtain optimized inter-critical annealing parameters, microstructure and superior combined mechanical properties of ductility and strength suitable for vehicle lightweight solution.
 - Meet DOE VTO MYPP targets and goals.
 - Help steel makers and users to expedite the development-to-deployment cycle

Milestone

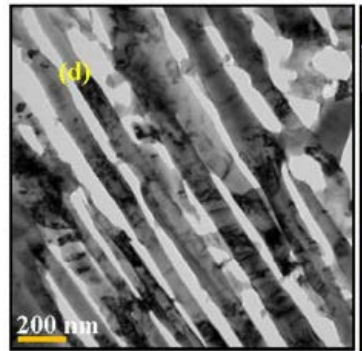
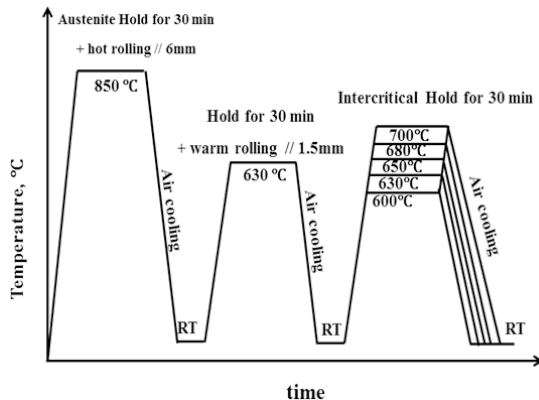
Date	Milestone or Go/No-go	Goal description	Status
9/30/2016	Milestone	Develop a high throughput HEXRD-based <i>in-situ</i> characterization process to obtain desired RA volume fraction and stability for 3rd GEN AHSS	Completed
9/30/2018	Milestone	A phase field modeling framework that can predict the effects of heat treatment parameters (i.e., IA temperature and time) on the phase volume fractions as well as C and Mn content in each phase	On track
9/30/2019	Milestone	An integrated modeling framework that can predict the effects of heat treatment parameters (i.e., IA temperature and time) on the ultimate tensile properties of 3rd GEN AHSS.	On track

Approach

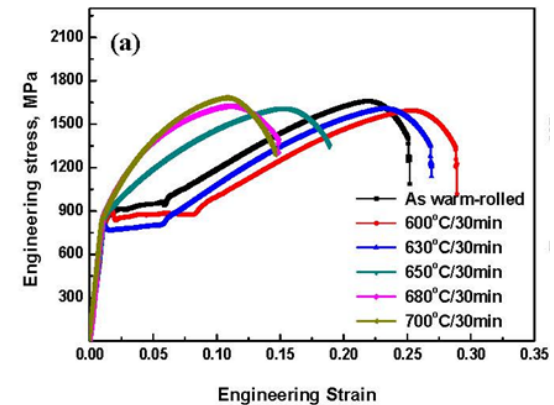


Medium Mn Steels & Heat Treatment Processes

- ▶ Med-Mn steel is an 3rd Gen AHSS which can have excellent combination of ductility and strength due to the austenite to martensite phase transformation during forming.
- ▶ Inter-critical annealing (IA) process after austenization is used to optimize the microstructure, esp. retained austenite volume fraction (RAVF).
- ▶ Both temperature and holding time affect the microstructure and RAVF leading to different strength and ductility of such steels.
- ▶ Ex-situ characterization is usually utilized after various heat treatment processing with different IA parameters, which is costly and time consuming
- ▶ An in-situ characterization during heat treatment processing can provide great opportunities to obtain full information of phase transformation during the whole process.



Fe-7.9Mn-0.14Si-0.05Al-0.07C Steel





Accomplishments to Date

- ▶ **High throughput *in-situ* HEXRD intercritical annealing (IA) heat treatment experiment** has been developed & utilized for three Med-Mn steels : 5Mn, 7Mn and 10Mn.
- ▶ *Ex-situ* heat treatment and characterization (SEM, HEXRD) has been completed on the Med-Mn steels.
- ▶ ThermoCalc-Dictra (TCD) simulations for 5Mn steels haven been developed to study phase transformation during IA holding.
- ▶ The Mn mobility (one of the thermodynamic parameter) in ferrite/martenite in ~5Mn steel has been determined by the proposed **integrated experimental (ex-situ & in-situ) and numerical modeling(TCD) framework**.
- ▶ Initial phase field microstructure modeling framework of 5Mn steel has been developed.
- ▶ Non incremental *In-situ* HEXRD tensile tests of 7Mn & 10Mn steels along different directions to better under the TRIP effect and the yield point elongations (Luders band behavior) of median Mn steels.
- ▶ **Microstructure/mechanism-based phenomenological and crystal plasticity FE models** have been developed with the consideration of martensitic transformation.
- ▶ Luders band and yield point elongation (YPE) behavior have been successfully captured by the above mentioned models.

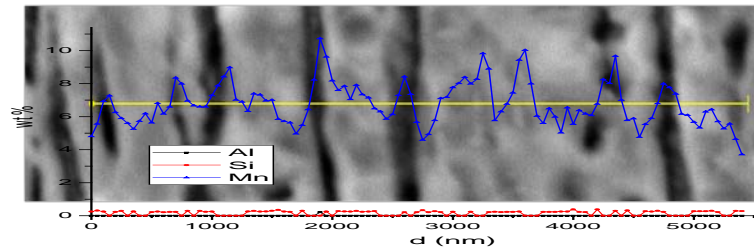
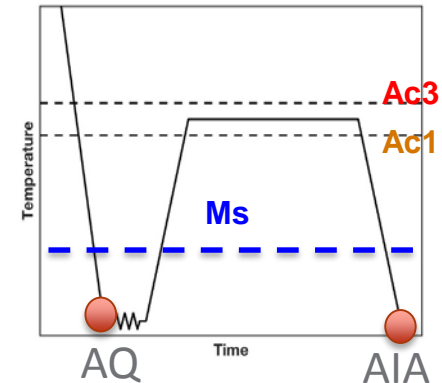
Accomplishments to Date

SEM-EDAX microstructural and composition analysis

- ▶ As-received: 7Mn, 10Mn steel (AIA)
- ▶ As-quenched (AQ) after full austenization: 5Mn steel

AQ 5Mn steel

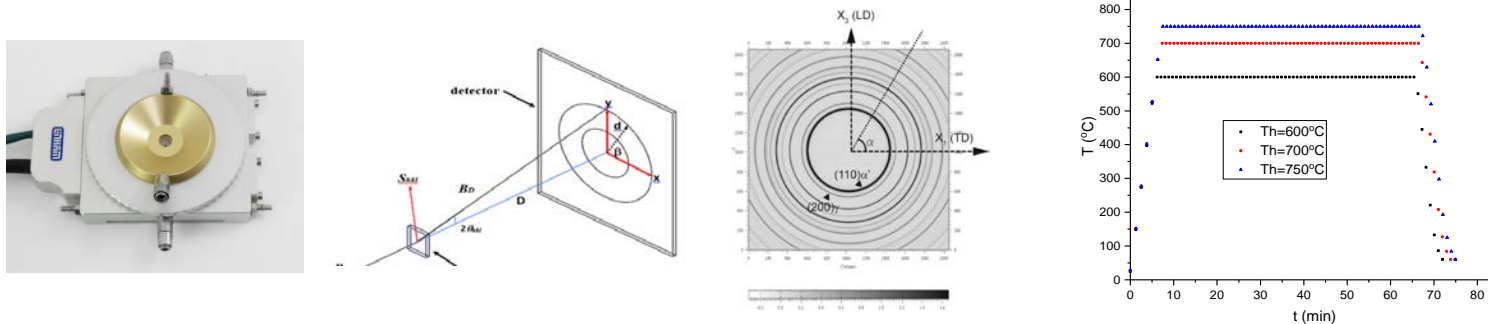
AIA 7Mn steel



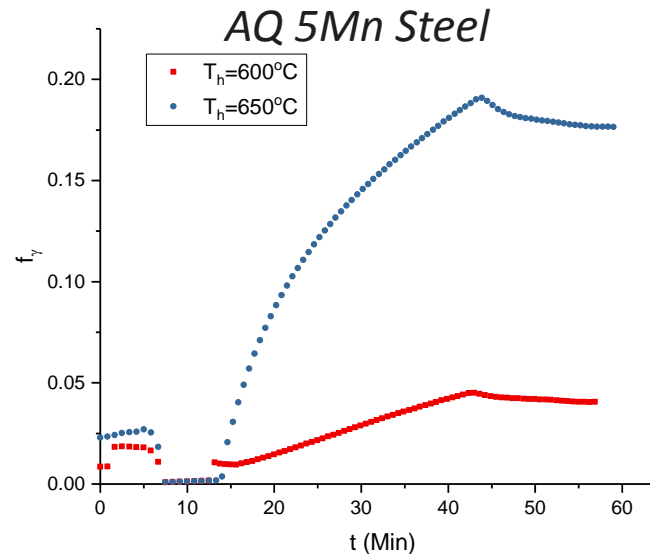
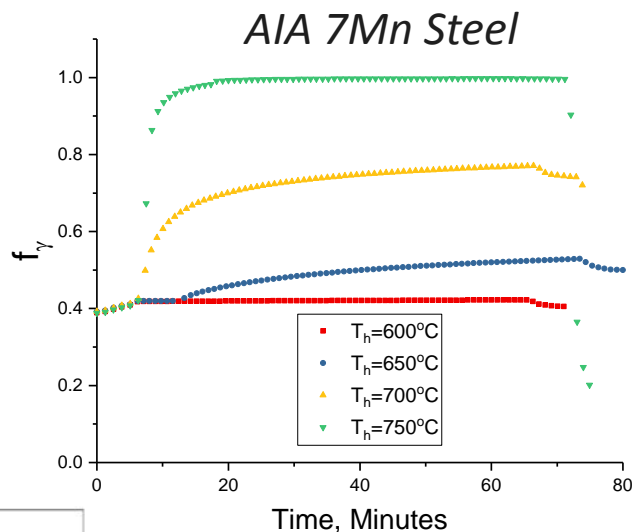
Accomplishments to Date

High Throughput In-situ HEXRD Test

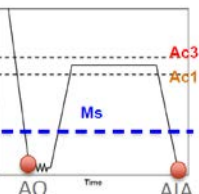
- ▶ The in-situ HEXRD IA experiments (APS beamline 11-ID-C).



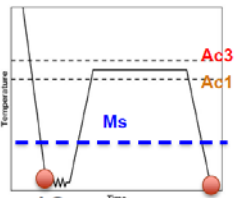
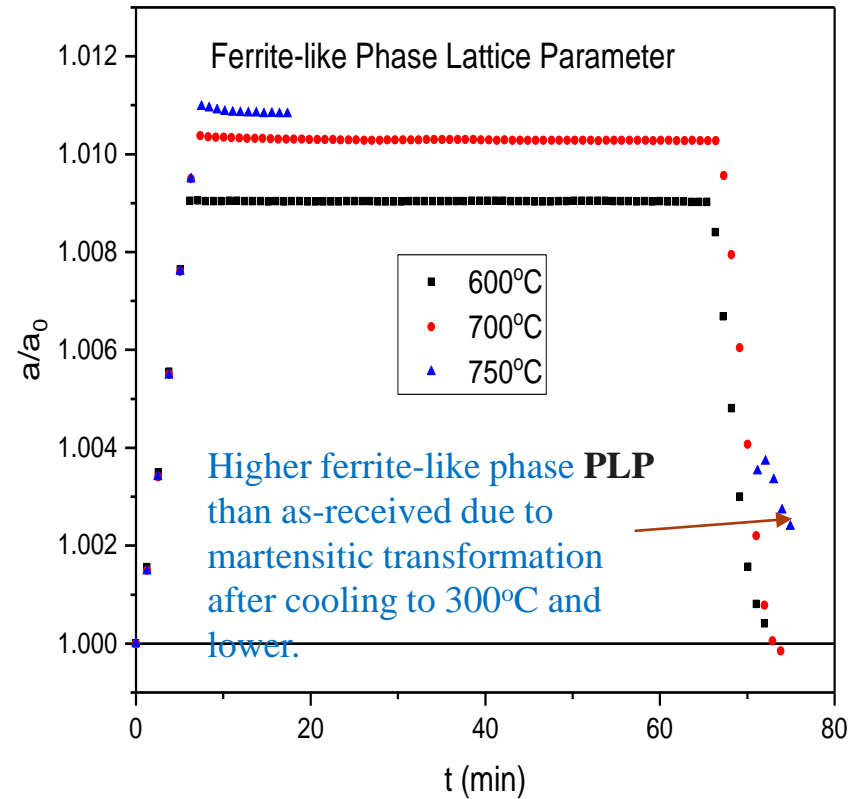
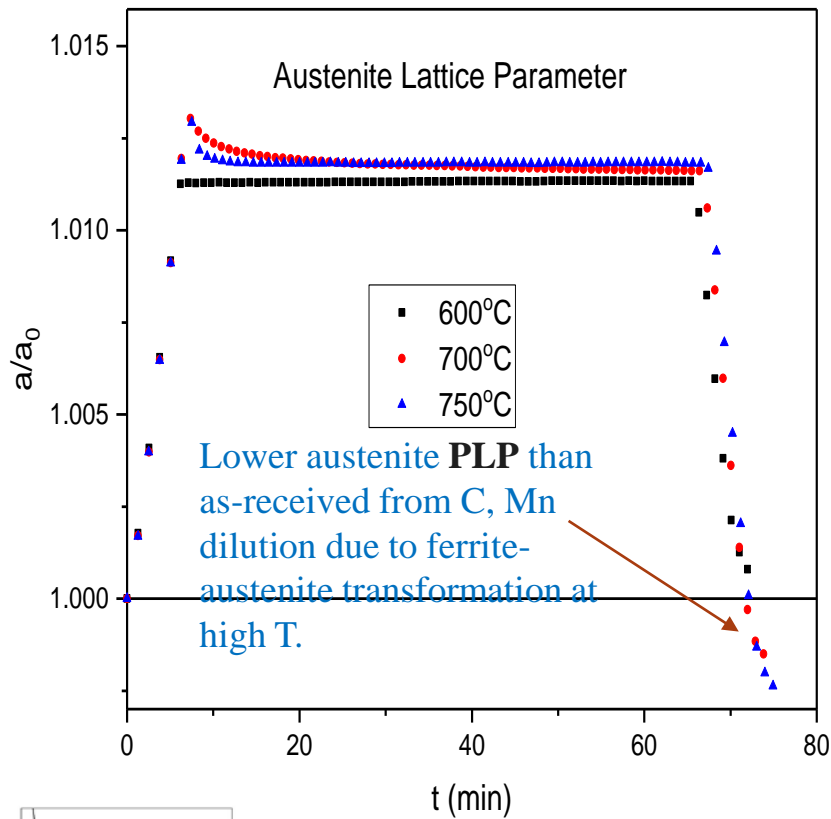
- ▶ Austenite volume fraction (AVF) as a function of t & T during IA



With conventional approach only the AVF at **RT** can be measured, the *in-situ* HEXRD method can provide AVF variation with **temperature (T)** and **time (t)**.



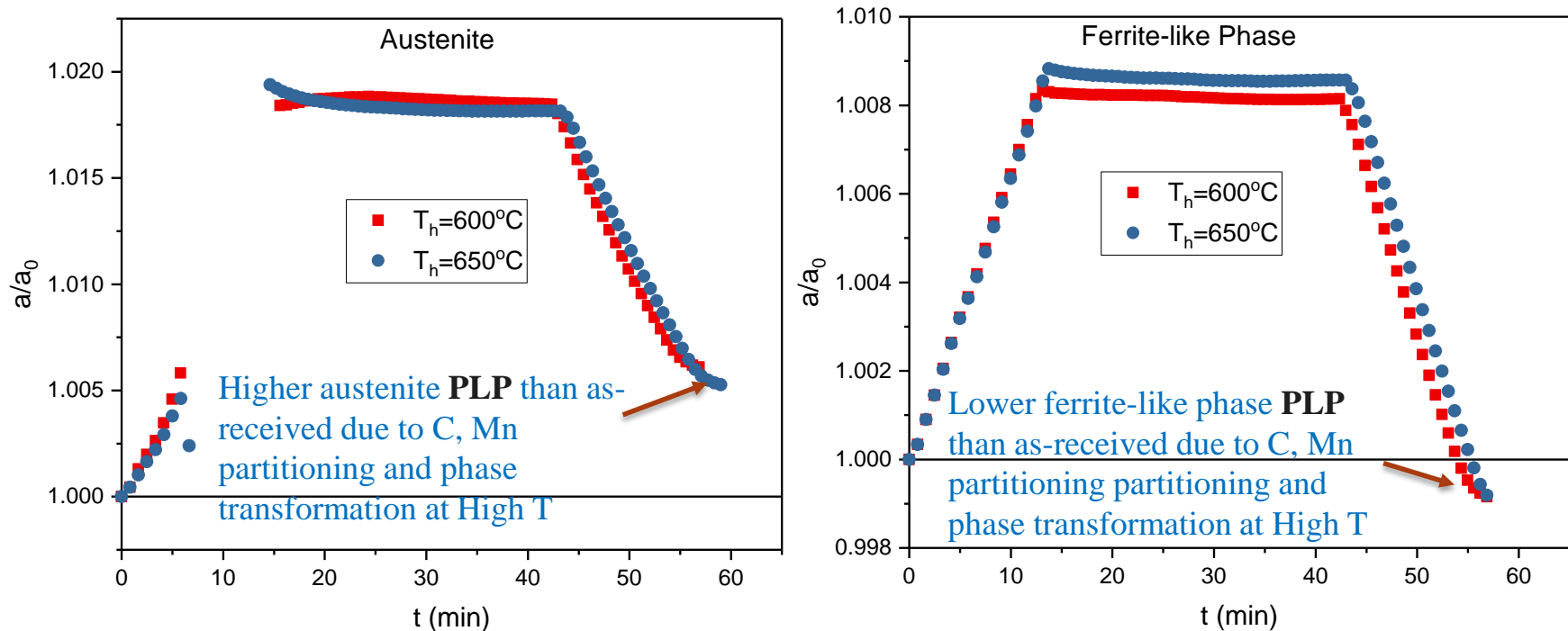
► Phase lattice parameter (PLP) change during IA (AIA 7Mn Steel)



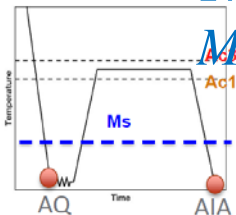
Accomplishments to Date

High Throughput In-situ HEXRD Test

► Phase lattice parameter change during IA (AQ 5Mn Steel)



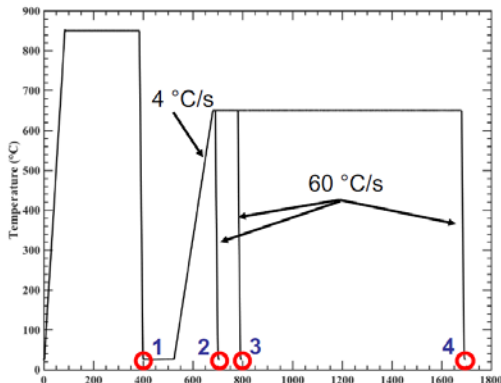
*The efforts of quantitatively linking **PLP** to alloy compositions (C, Mn) is still under progress*



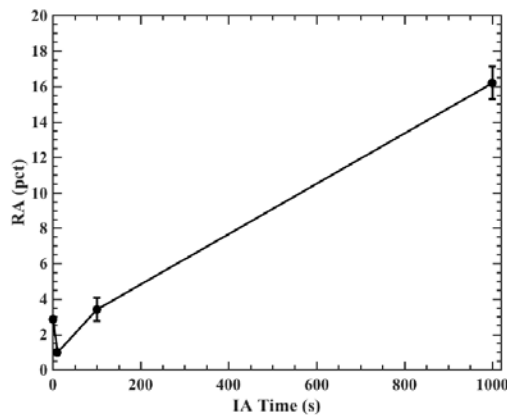
Accomplishments to Date

Ex-Situ heat treatment and characterization (SEM-EDAX) has been performed on 5Mn steels

- ▶ Initial Material: 0.19C-4.39Mn, Hot-rolled+Annealed+Cold Rolled
- ▶ Heat Treatment:

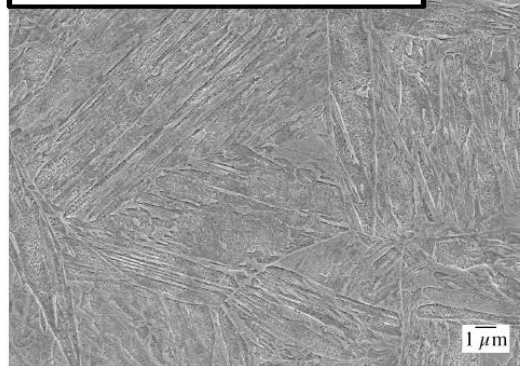


- ▶ AVF measured by HEXRD after IA

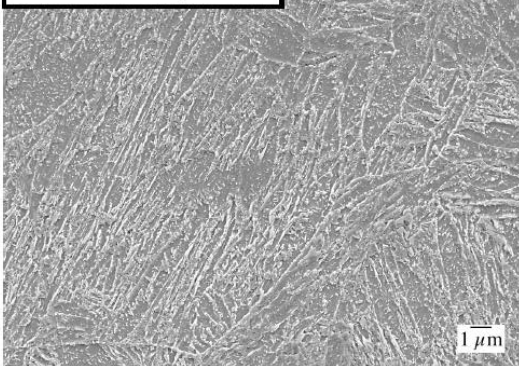


- ▶ Microstructure after IA

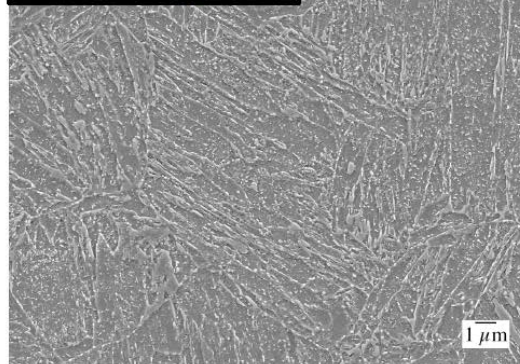
Austenitized + Quenched



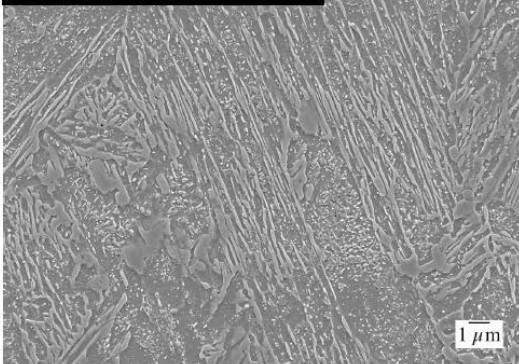
IA: 650 °C, 10 s



IA: 650 °C, 100 s



IA: 650 °C, 1000 s



ThermoCal-Dictra (TCD) Microstructural Modeling¹

- ▶ 0.2-4.39Mn
- ▶ One dimension model



- ▶ Modeling the microstructure change during holding
 - Pre-simulation condition: AQ + heating to holding temperature
 - Initial cell sizes: γ -0.05 nm, α -208.5nm (no initial austenite)
 - Initial Composition: γ -0.2 C-4.39Mn, α -0.001 C-4.39Mn

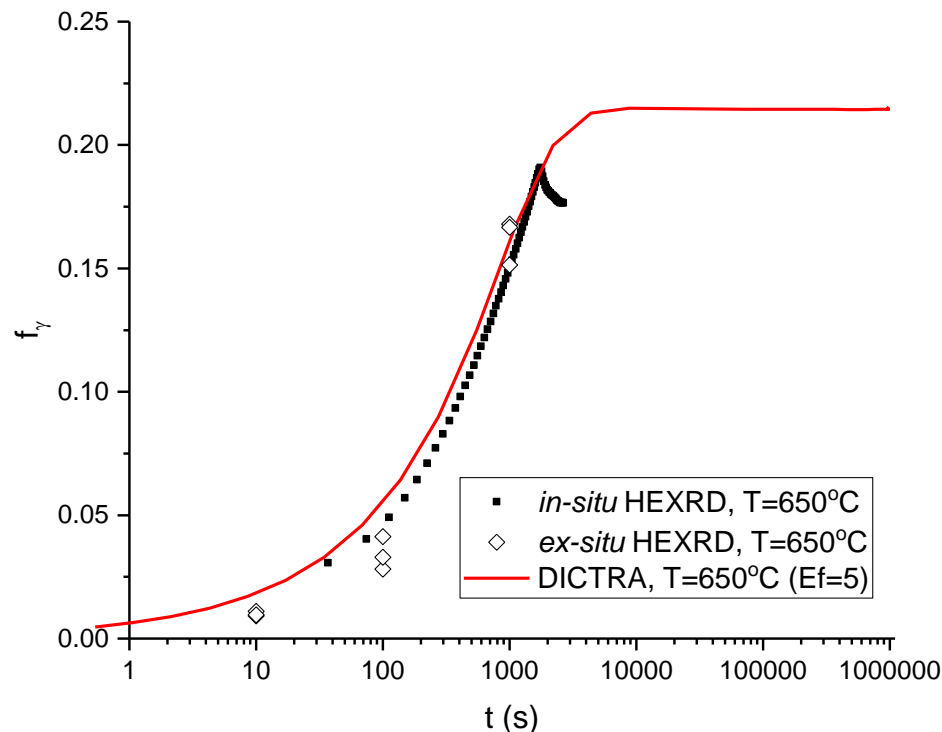
The one-dimension TCD model is a good approximation for the lath-like microstructures



¹ Mueller et al., Proceedings of MST 2017.

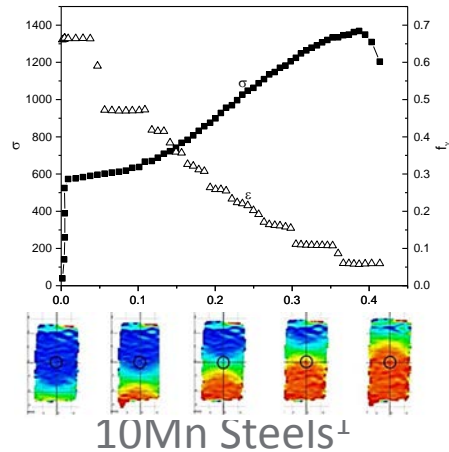
Determination of Mn Mobility by TCD and in-situ HEXRD data

- Mn Mobility enhancement factor (E_f) has been calibrated to be 5 by proposed **integrated framework**: Iteratively comparing the simulated AVF as a function with time ($T_h=650^\circ\text{C}$) with that of in-situ & ex-situ HEXRD measurement results.



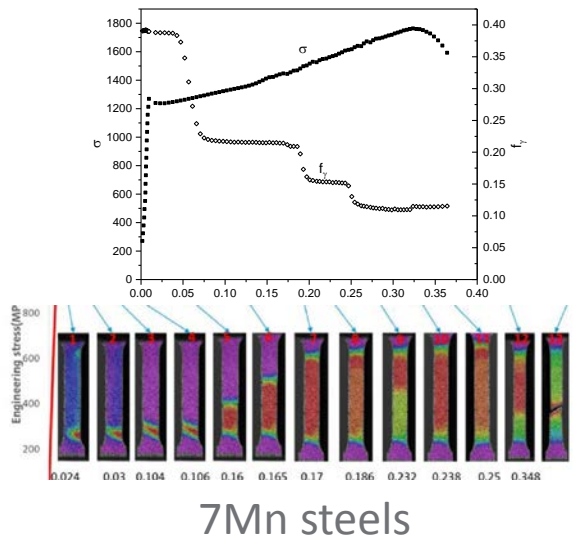
In TCD database, there is only Mn mobility (M_{Mn}^f) data in ferrite. The mobility enhancement factor can be used in TCD to modify the ferrite Mn mobility data to represent the martensite phase.

Deformation Mechanism of Med-Mn Steels: Luders band and YPE



- ▶ Step-wise transformation¹
- ▶ Mechanisms of Luders band and YPE^{1,2}
 - Bain Transformation strain?
 - Very high dislocation density (Huang)³ ?

1. Abu-Farha, Hu, Sun & Hector, Mat Met Trans A, submitted (2018)
2. Sun et al., AIST conference (2017)
3. Huang, et al., Science (2017)



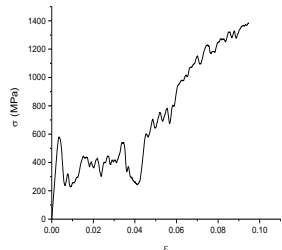
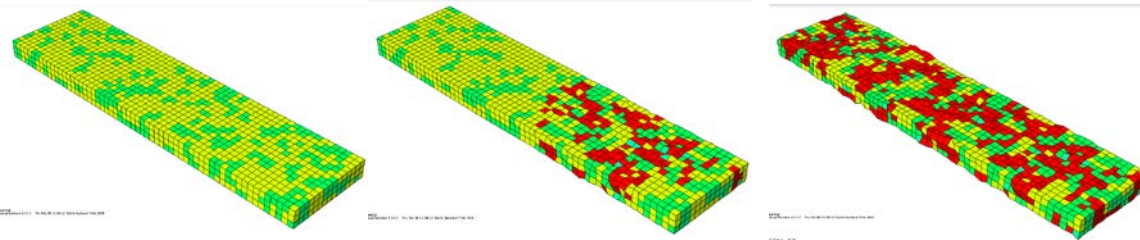
YPE: Yield Point Elongation

Accomplishments to Date

Modeling Luders Band from Microstructure-based

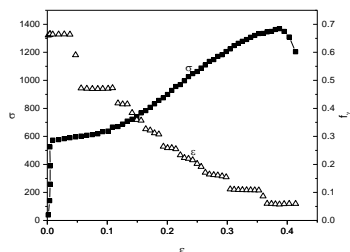
- ▶ Luders Band & YPE is captured by considering Bain strain during transformation

- Crystal plasticity (CP) finite element (FE) model
- FE Model assuming J2 plasticity

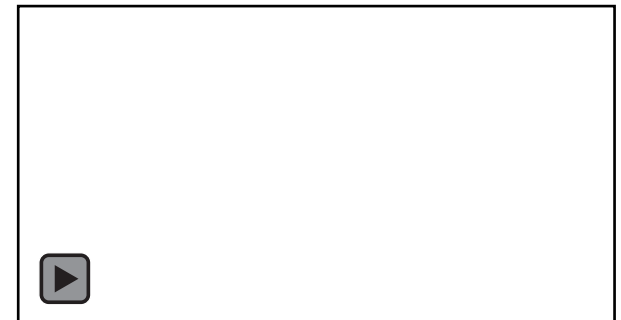


This is the initial attempt, more comprehensive studies will be performed in the future used the slip system parameters (SP) determined by the HEXRD-CP approach ^{1,2}.

1. Hu, Choi, Sun, et al. Mat Met. Trans. A (2016)
2. Hu, Sun, Hector, Ren, Acta Mat. (2017)



CP-FE model video



FE-model assuming J2 plasticity video

Responses to Previous Years Reviewers' Comments

- ▶ Reviewer: The objective needs to be defined in a clearer definitive manner
 - Answer: In the present presentation, the objective has been clearly defined.
- ▶ Reviewer: The technical accomplishments are not clearly correlated to the 3GAHSS mission
 - Answer: The optimization of heat treatment process is the key to the success to produce 3GAHSS which has optimized microstructure and properties suitable for vehicle light-weighting. In our last AMR period, we have met the required milestone which is in-line with our eventual objectives.
- ▶ The reviewer: There is a good mix of national laboratories and academia, but added the project would benefit from more industrial (OEM and supplier (steel company) collaboration.
 - Answer: Thanks. The ASPPRC is a researcher center which act as interface between steel makers and users.
- ▶ The reviewer: The future research is not clearly defined
 - Answer: In the present presentation, the future research is clearly stated.

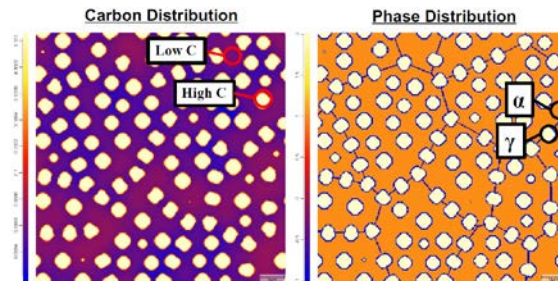


Collaboration and Coordination

- ▶ Computational Engineering Group (CEG), Pacific Northwest National Laboratory (PNNL)
 - High throughput In-situ HEXRD heat treatment experiments and characterization
 - Mechanism/microstructure-based finite element modeling of the TRIP assisted 3G AHSS steel with the aid of in-situ HEXRD tensile tests.
- ▶ Advanced Steels Processing and Products Center (ASPPRC), Colorado School of Mines (CSM)
 - Ex-situ heat-treatment experiments & materials characterization
 - Microstructural modeling during heat treatment process
- ▶ Energy and Transportation Science Division, Oak Ridge National Laboratory (ORNL)
 - Advisory
- ▶ Advanced Photon Source (APS), Argonne National Laboratory (ANL)
 - In-situ HEXRD beamline user facility and in-situ HEXRD experiments assistance.

Remaining Challenges and Barriers

- ▶ Obtaining accurate chemical compositions from phase lattice parameters (PLP).
 - Lack of accurate models accounting for both temperature & composition impacts.
- ▶ TCD models is unable to model diffusion less martensitic transformation during quenching, phase field model is required.
- ▶ Accurate phase field microstructure/phase transformation modeling of the whole heat treatment processes of phase transformation and C, Mn partitioning.
 - We are in the initial stages of developing models for Med-Mn 3G AHSS.



- ▶ Accurate mechanism/microstructure-based modeling of Med-Mn 3G AHSS.
 - We have achieved initial success on qualitatively capturing luders band behavior by the consideration of Bain strain. More accurate models (including kinematic hardening) and comprehensive studies are needed.



Proposed Future Work

- ▶ Continue the study on correlating phase lattice parameter changes with chemical composition change during IA heat treatment process.
- ▶ Continue the development of a phase field model which will be able to used for
 - Accurate determinations of thermodynamic parameters with the help from the in-situ & ex-situ experimental techniques.
- ▶ Continue the development of mechanism/microstructure-based modeling of Med-Mn 3G AHSS mechanical performance during forming.
- ▶ Using the information of the correlation between microstructure and mechanical performance, determine optimized IA parameters to obtain desired microstructures using TCD/phase field based modeling.

Any proposed future work is subject to change based on funding levels



Summary

- ▶ SEM-EDAX microstructural and composition analysis has been performed on as-received 7Mn and 10Mn steels to obtain information of Mn, Al, Si partitioning in austenite and ferrite phases.
- ▶ Ex-Situ heat treatment and characterization (SEM-EDAX) has been performed on 5Mn steels.
- ▶ High throughput *in-situ* HEXRD measurement technique has been developed & used to obtain AVS and PLP during inter-critical annealing (IA) cycles of 5Mn (as-quenched), 7Mn and 10Mn (as-received) steels.
- ▶ ThermoCalc-Dictra (TCD) simulations for 5Mn steels (as-quenched) haven been performed to study martensitic transformation and C, Mn partitioning during IA holding.
- ▶ The Mn mobility in Ferrite/martensite in 5Mn steel has been determined by integrated HEXRD AVS measurements and TCD microstructure modeling.
- ▶ Phase field microstructure modeling of 5Mn steel has been started.
- ▶ Non incremental *In-situ* HEXRD tensile tests of 7Mn & 10Mn steels along different directions to better understand the TRIP effect and the yield point elongations (Luders band behavior) of medium Mn steels.
- ▶ Phenomenological and Crystal plasticity FE models have been established with the consideration of martensitic transformation and the Luders band and yield point elongation (YPE) has been successfully captured by the models.